



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:10 PM GMT

PDB ID : 1J36  
Title : Crystal Structure of Drosophila AnCE  
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Deposited on : 2003-01-20  
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

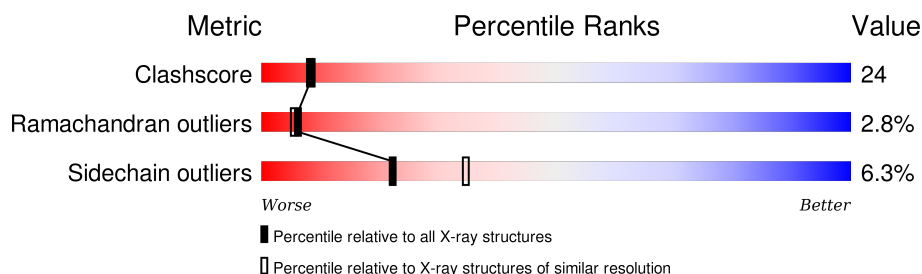
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	607	 58% 35% 5% •
1	B	607	 57% 36% 6% •

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10263 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called angiotensin converting enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	598	Total	C	N	O	S	154	0	0
			4900	3135	819	926	20			
1	B	598	Total	C	N	O	S	154	0	0
			4900	3135	819	926	20			

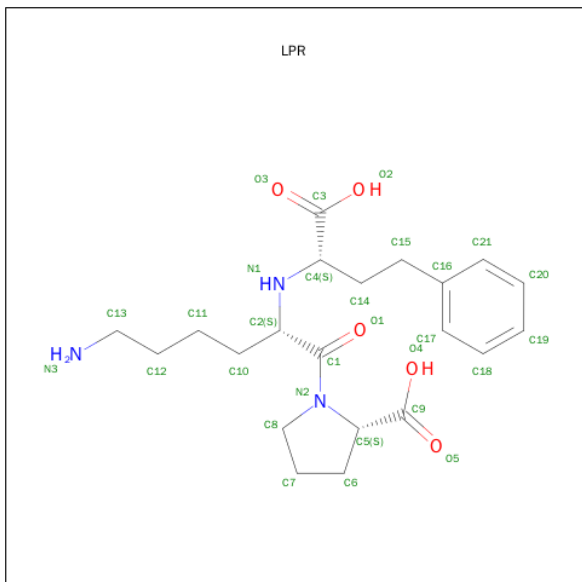
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	ARG	GLY	CONFLICT	UNP Q10714
A	53	ALA	ASN	CONFLICT	UNP Q10714
A	607	ILE	THR	CONFLICT	UNP Q10714
A	616	HIS	-	EXPRESSION TAG	UNP Q10714
A	617	HIS	-	EXPRESSION TAG	UNP Q10714
A	618	HIS	-	EXPRESSION TAG	UNP Q10714
A	619	HIS	-	EXPRESSION TAG	UNP Q10714
A	620	HIS	-	EXPRESSION TAG	UNP Q10714
B	51	ARG	GLY	CONFLICT	UNP Q10714
B	53	ALA	ASN	CONFLICT	UNP Q10714
B	607	ILE	THR	CONFLICT	UNP Q10714
B	616	HIS	-	EXPRESSION TAG	UNP Q10714
B	617	HIS	-	EXPRESSION TAG	UNP Q10714
B	618	HIS	-	EXPRESSION TAG	UNP Q10714
B	619	HIS	-	EXPRESSION TAG	UNP Q10714
B	620	HIS	-	EXPRESSION TAG	UNP Q10714

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is [N2-[(S)-1-CARBOXY-3-PHENYLPROPYL]-L-LYSYL-L-PROLINE (three-letter code: LPR) (formula: C<sub>21</sub>H<sub>31</sub>N<sub>3</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			29	21	3	5		
3	B	1	Total	C	N	O	0	0
			29	21	3	5		

- Molecule 4 is water.

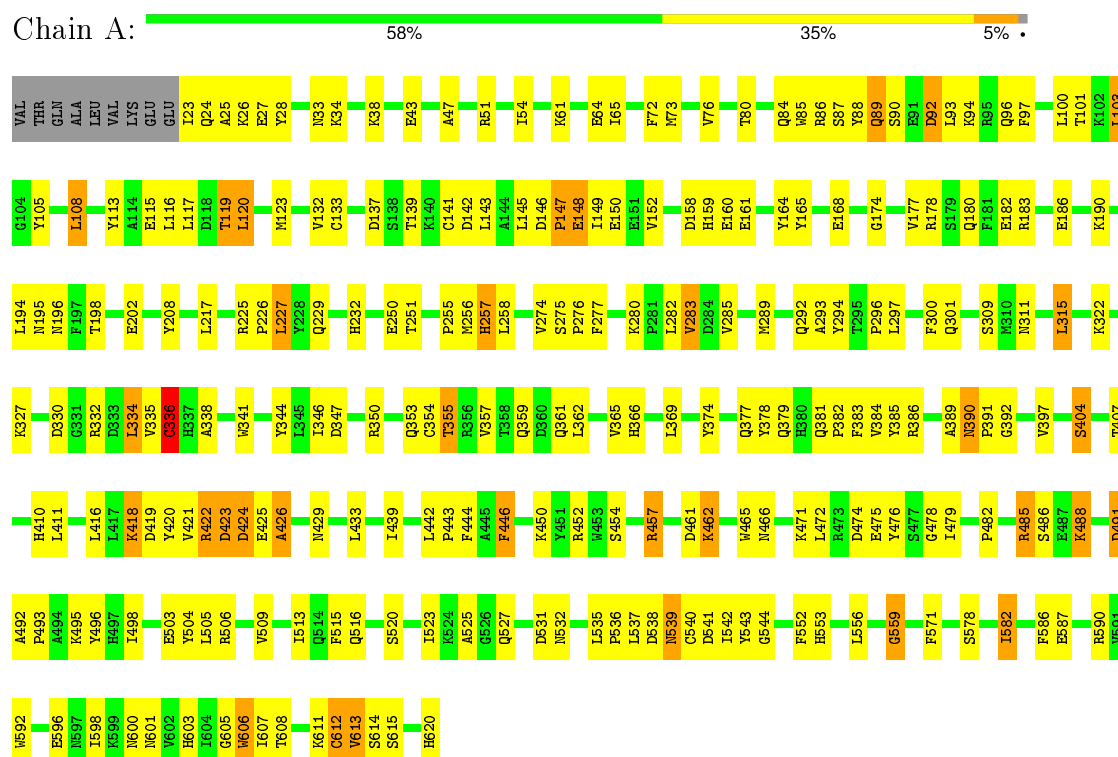
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	196	Total	O	0	0
			196	196		
4	B	207	Total	O	0	0
			207	207		

### 3 Residue-property plots

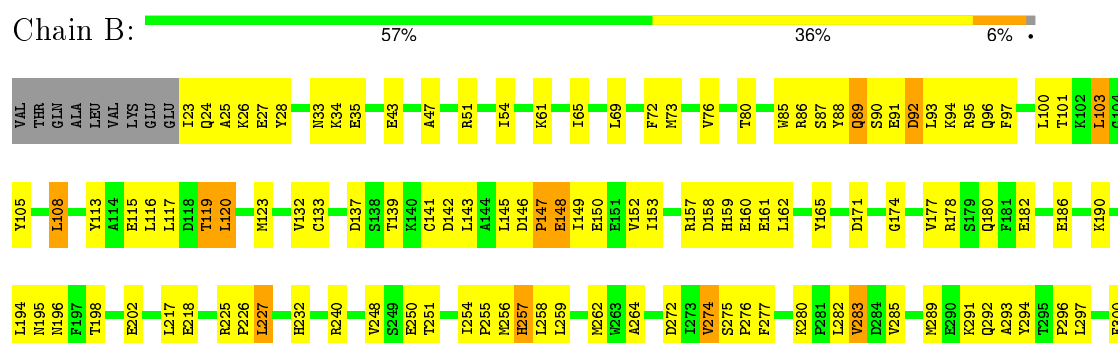
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: angiotensin converting enzyme



- Molecule 1: angiotensin converting enzyme



Q301	A389	R485	M577
S309	M390	S486	S578
M310	P391	E487	I582
N311	G392	K488	A583
L315	V397	D491	E584
K322	S404	A492	Y585
K327	T407	P493	F586
D330	K410	A494	E587
G331	H411	K495	R590
R332	L411	Y496	W591
L334	L416	H497	W592
V335	L417	I498	E596
C336	K418	E503	M600
W341	D419	Y504	L601
D342	R422	L505	W602
F343	D423	R506	H603
E425	D424	L508	L604
Y344	E426	Y509	G605
L345	A426	I513	W606
L346	M429	G514	I607
D347	L433	F515	T608
R350	I439	Q516	C612
Q353	I442	S520	V613
C354	P443	I523	S614
T355	F446	R524	S615
V357	D449	A525	H620
T358	K450	R526	
R360	Y461	Q527	
Q361	W463	Y528	
L362	S454	D531	
V365	R457	H532	
H366	D461	L535	
L369	K462	P536	
Y374	W465	L537	
F375	L472	D538	
L376	R473	H539	
Q377	D474	C540	
Y378	E475	D541	
Q379	Q381	I542	
H380	Y476	Y543	
Q382	S477	G544	
F383	G478	F552	
Y384	I479	H553	
Y385	P482	L556	
R386		G559	
		F571	

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.91Å 121.22Å 94.74Å 90.00° 99.39° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	92.2 (20.00-2.40)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.234 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10263	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, LPR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.45	0/5031	0.67	3/6814 (0.0%)
1	B	0.46	0/5031	0.67	3/6814 (0.0%)
All	All	0.46	0/10062	0.67	6/13628 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	CYS	CA-CB-SG	-5.85	103.47	114.00
1	A	457	ARG	N-CA-C	-5.68	95.65	111.00
1	B	457	ARG	N-CA-C	-5.57	95.96	111.00
1	B	336	CYS	CA-CB-SG	-5.35	104.36	114.00
1	B	491	ASP	N-CA-C	5.17	124.97	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4900	0	4696	217	0
1	B	4900	0	4696	240	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	29	0	29	1	0
3	B	29	0	29	1	0
4	A	196	0	0	10	0
4	B	207	0	0	31	0
All	All	10263	0	9450	458	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

The worst 5 of 458 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:LYS:HE2	1:B:93:LEU:HD21	1.39	1.03
1:B:479:ILE:HA	4:B:947:HOH:O	1.57	1.01
1:A:26:LYS:HE2	1:A:93:LEU:HD21	1.40	0.98
1:B:347:ASP:H	1:B:379:GLN:NE2	1.68	0.92
1:A:347:ASP:H	1:A:379:GLN:NE2	1.67	0.91

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	596/607 (98%)	541 (91%)	39 (6%)	16 (3%)	<b>6</b> <b>6</b>
1	B	596/607 (98%)	537 (90%)	42 (7%)	17 (3%)	<b>6</b> <b>5</b>
All	All	1192/1214 (98%)	1078 (90%)	81 (7%)	33 (3%)	<b>6</b> <b>5</b>

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	ASP
1	A	147	PRO
1	A	423	ASP
1	A	424	ASP
1	A	542	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	522/530 (98%)	490 (94%)	32 (6%)	23	36
1	B	522/530 (98%)	488 (94%)	34 (6%)	21	33
All	All	1044/1060 (98%)	978 (94%)	66 (6%)	22	35

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	601	ASN
1	B	119	THR
1	B	537	LEU
1	A	606	TRP
1	B	100	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	539	ASN
1	B	41	ASN
1	B	532	ASN
1	A	600	ASN
1	A	610	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	LPR	A	801	2	24,30,30	1.93	8 (33%)	24,39,39	1.00	1 (4%)
3	LPR	B	802	2	24,30,30	1.97	11 (45%)	24,39,39	1.00	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LPR	A	801	2	-	0/22/40/40	0/2/2/2
3	LPR	B	802	2	-	0/22/40/40	0/2/2/2

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	LPR	C7-C6	-3.51	1.36	1.51
3	A	801	LPR	C7-C6	-3.48	1.37	1.51
3	A	801	LPR	C19-C18	2.03	1.43	1.38
3	B	802	LPR	C19-C18	2.06	1.43	1.38
3	B	802	LPR	C18-C17	2.10	1.43	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	LPR	C6-C7-C8	2.87	113.46	105.22
3	B	802	LPR	C6-C7-C8	2.99	113.81	105.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	LPR	1	0
3	B	802	LPR	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.